Crystal structure of ethylenediammonium-*N,N′*-di-3-propionic acid tetrachloroplatinate(II), $(CH_2NH_2(CH_2)_2COOH)_2[PtCl_4]$

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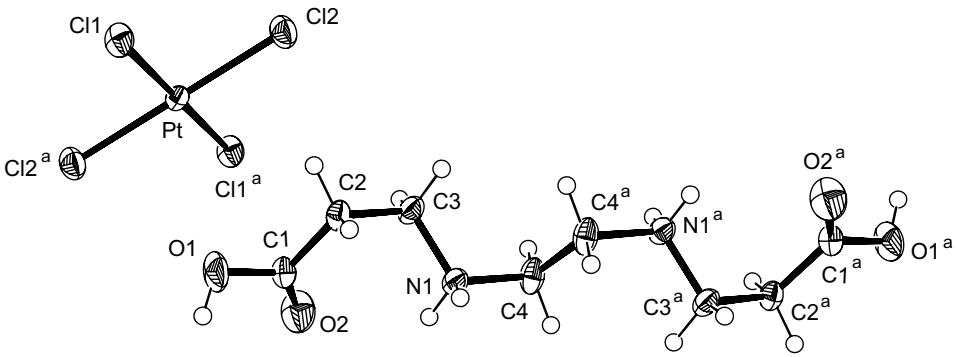
Received June 22, 2006, accepted and available on-line August 28, 2006; CCDC no. 1267/1822



Abstract

$C_8H_{18}Cl_4N_2O_4Pt$, monoclinic, $P12_1/n1$ (no. 14), a = 8.181(3) Å, b = 10.303(5) Å, c = 9.073(6) Å, β = 103.2(1)°, V = 744.6 Å^3, Z = 2, $R_{gt}(F)$ = 0.080, $wR_{ref}(F^2)$ = 0.247, T = 293 K.

Source of material

Potassium tetrachloroplatinate(II) (0.200 g, 0.482 mmol) and ethylenediamine-*N,N′*-di-3-propanoic acid dihydrochloride (0.133 g, 0.482 mmol) were dissolved in 20 ml of water. The reaction mixture was left at room temperature for a few days. After one week, orange crystals were formed from the mother liquor. Upon crystallization crystals were filtered off.

Experimental details

The relatively large *R* values can be explained by rather bad quality of single crystals.

Discussion

Only one crystal structure with the ethylenediammonium-*N,N′*-di-3-propanoic acid cation counter to a metal complex anion is described in the literature, (ethylenediammonium-*N,N′*-di-3-propanoic acid) tetrachloropalladate(II) complex [1], $H_4eddp[PdCl_4]$. The title complex consists of two entities: the anion $[PtCl_4]^{2-}$ and dication H_4eddp^{2+}. The $[PtCl_4]^{2-}$ anion exhibits a square-planar coordination with slight deviations from ideal values of 90° with respect to *cis*-coordinated Cl atoms. The H_4eddp^{2+} ion is nearly linear. The β-alaninate part of the cation forms *gauche* conformation (∠N1–C3–C2–C1 = –64.9(8)°). The C4–N1–C3–C2 torsion angle of –171(1)° shows a nearly *antiperiplanar* conformation of the H_4eddp^{2+} ion. Deviation in the Cl–Pt–Cl angle can be explained by intermolecular hydrogen bond interactions between N1–H1···Cl1. Structural fragment –C(3)H_2–C(2)H_2–C(1)OOH is nearly planar and its plane is parallel with the $[PtCl_4]$ coordination plane. Every $[PtCl_4]$ species is located between two above-mentioned fragments. It is interesting to note that one of two H atoms from the C(2)H_2 group is directed to the Pt atom occupying approximately axial position. The Pt—H distance is 3.012(2) Å that is shorter than sum of the van der Waals radii. The C2–H···Pt angle is 127.2(5)°. In this way the Pt atom is situated in a deformed octahedral surrounding formed by four equatorial Cl and two H atoms located on the axial positions. Isostructural complexes, $H_4eddp[PtCl_4]$ and $H_4eddp[PdCl_4]$, have nearly equal *M—L* bond distances and corresponding angles. This is in agreement with the ionic radii of the central atom.

Table 1. Data collection and handling.

Crystal:	orange prism, size 0.12 × 0.56 × 0.56 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	101.50 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, $\omega/2\theta$
$2\theta_{max}$:	52°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1562, 1461
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1332
$N(param)_{refined}$:	89
Programs:	SHELXS-97 [2], SHELXL-97 [3], ORTEP-3 [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1N1)	4*e*	0.7005	0.4124	–0.0292	0.029
H(2N1)	4*e*	0.8499	0.3334	0.0211	0.029
H(1O1)	4*e*	0.4129	0.1557	0.1701	0.062
H(22)	4*e*	0.7225	0.3320	0.3569	0.029
H(12)	4*e*	0.7771	0.2411	0.2384	0.029
H(13)	4*e*	0.7312	0.5103	0.1973	0.031
H(23)	4*e*	0.9077	0.4448	0.2523	0.031
H(24)	4*e*	0.8837	0.5104	–0.1407	0.035
H(14)	4*e*	0.8814	0.5996	–0.0006	0.035

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pt	2*b*	½	½	½	0.0256(6)	0.0139(6)	0.0206(7)	0.0008(1)	0.0095(4)	–0.0013(1)
Cl(1)	4*e*	0.5805(2)	0.3380(2)	0.6767(2)	0.034(1)	0.021(1)	0.035(1)	–0.0005(7)	0.0075(8)	0.0094(7)
Cl(2)	4*e*	0.7682(2)	0.5845(2)	0.5517(2)	0.030(1)	0.031(1)	0.038(1)	–0.0073(8)	0.0068(9)	0.0060(7)
N(1)	4*e*	0.8053(8)	0.4122(6)	0.0294(7)	0.033(3)	0.019(3)	0.023(3)	–0.005(3)	0.011(3)	–0.001(2)
O(1)	4*e*	0.4617(9)	0.2062(7)	0.2353(8)	0.039(3)	0.040(4)	0.045(4)	–0.014(3)	0.012(3)	0.017(3)
O(2)	4*e*	0.4560(9)	0.3641(7)	0.0647(8)	0.042(3)	0.048(4)	0.051(4)	0.002(3)	0.009(3)	0.019(3)
C(1)	4*e*	0.5329(9)	0.2994(7)	0.1711(9)	0.022(3)	0.017(3)	0.030(4)	0.002(3)	0.009(3)	0.004(3)
C(2)	4*e*	0.715(1)	0.3192(7)	0.2497(9)	0.026(3)	0.022(3)	0.027(4)	–0.001(3)	0.012(3)	0.002(3)
C(3)	4*e*	0.796(1)	0.4323(8)	0.1902(9)	0.035(4)	0.023(3)	0.024(4)	–0.004(3)	0.015(3)	–0.004(3)
C(4)	4*e*	0.909(3)	0.514(1)	–0.031(3)	0.033(8)	0.020(5)	0.040(8)	0.002(4)	0.020(6)	0.006(5)

Acknowledgment. The authors are grateful to the Ministry of Science and Environmental Protection of the Republic of Serbia for financial support (grant no. 142010).

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